

Instanton calculation of the density of states of disordered Peierls chains

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(February 7, 2008)*

We use the optimal fluctuation method to find the density of electron states inside the pseudogap in disordered Peierls chains. The electrons are described by the one-dimensional Dirac Hamiltonian with randomly varying mass (the Fluctuating Gap Model). We establish a relation between the disorder average in this model and the quantum-mechanical average for a certain double-well problem. We show that the optimal disorder fluctuation, which has the form of a soliton-antisoliton pair, corresponds to the instanton trajectory in the double-well problem. We use the instanton method developed for the double-well problem to find the contribution to the density of states from disorder realizations close to the optimal fluctuation.

I. INTRODUCTION

In studies of disordered systems, one often encounters the problem of finding the density of single-particle states in energy regions where the states can only exist as a consequence of disorder. An example is the density of negative energy states of a particle moving in a random potential (the lowest energy of a free particle is zero).^{1–3} Another example is provided by a superconductor with magnetic impurities. The impurities break Cooper pairs and fill the gap with electron states of arbitrarily small energy.⁴ The density of such states (“Lifshitz tails”) is typically small, as it requires a large disorder fluctuation to induce them. In that case the density can be estimated by the probability of the least suppressed disorder fluctuation that creates a state of a given energy (the so-called optimal fluctuation method).^{1–4}

In Ref. 5 we applied the optimal fluctuation method to study the density of states and optical absorption in disordered Peierls insulators. In the absence of disorder, the electron excitation spectrum in these quasi-one-dimensional materials has a gap which results from the electron-lattice instability and is accompanied by a periodic lattice distortion with the wave vector $Q = 2k_F$.⁶ We considered half-filled chains, in which case the Peierls instability results in an alternation of long and short bonds (dimerization). Disorder in the electron hopping amplitudes induces electron states inside the Peierls gap, transforming it into a pseudogap. In Ref. 5 we showed that the optimal fluctuation for a disordered dimerized chain has the form of a soliton-antisoliton pair. It induces two electron states which lie close to the center of the pseudogap and which are symmetric and antisymmetric superpositions of states localized near the soliton and antisoliton. Knowing the typical form of the disorder-induced electron states we were able to find the absorption coefficient at small energies. These results were also used to explain the coexistence of the dimerization and antiferromagnetism, observed recently in the spin-Peierls material CuGeO₃.⁷

The probability of the optimal configuration gives, however, only an estimate of the density of states. A more careful calculation requires finding the contribution of disorder realizations close to the optimal one. In this paper, we perform such a calculation using the close relation between the optimal fluctuation method and the semiclassical approximation in quantum mechanics and field theory. In the path integral version of this approximation, the most important paths lie close to the “saddle-points” of the action, called instantons.^{8,9} In particular, the instantons for the double-well problem are the classical trajectories describing the imaginary time motion between the two wells, which corresponds to tunneling and results in level splitting. We show how the disorder average of the density of states can be written in the form of a functional integral that represents the sum over all paths of a particle in a corresponding double-well potential. Then the optimal disorder configuration becomes precisely the instanton trajectory and the calculation of the density of states can be done using standard instanton methods.

The outline of this paper is as follows. In Sec. II we introduce the Fluctuating Gap Model describing disordered Peierls systems and briefly discuss the previously obtained analytical results for the disorder-averaged density of states in that model. Next, in Sec. III we establish the relation between the disorder average in the Fluctuating Gap Model and the quantum-mechanical average for a certain double-well problem. We find the instanton trajectory corresponding to the optimal fluctuation and perform the

“saddle-point” integration for the average density of states. We discuss our results and conclude in Sec. IV. Two technical points are addressed in appendices. In Appendix A we discuss how the symmetries of the FGM Hamiltonian are crucial for the validity of the optimal fluctuation method. In Appendix B we discuss the instanton calculation for a different choice of boundary conditions.

II. THE FLUCTUATING GAP MODEL

The Fluctuating Gap Model (FGM) is a continuum model describing electrons in disordered quasi-one-dimensional semiconductors.^{10,11} In this paper we use it to describe half-filled Peierls chains with disorder in the hopping amplitudes of the electrons between the chain’s lattice sites. These systems are characterized by the Peierls order parameter, $\Delta(x)$, which is the (continuum version of the) alternating part of the hopping amplitudes along the chain, *i.e.*, the difference between the hopping amplitudes on nearest odd and even bonds. In the absence of disorder this order parameter (also called “dimerization”) is constant along the chain and equals the gap in the single-electron spectrum.^{6,12} Disorder in the electron hopping amplitudes results in random variations of the order parameter along the chain (which explains the name of the model):

$$\Delta(x) = \Delta_0 + \eta(x) . \quad (1)$$

Here, Δ_0 is the average value of the order parameter and $\eta(x)$ is the fluctuating part with a Gaussian correlator,

$$\langle \eta(x) \eta(y) \rangle = A \delta(x - y) . \quad (2)$$

The single-electron states close to the Fermi energy $\varepsilon_F = 0$, are described by the wave function

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} ,$$

where the two amplitudes $\psi_1(x)$ and $\psi_2(x)$ correspond to electrons moving, respectively, to the right and to the left with the Fermi velocity v_F . Since the density of single-electron states does not depend on spin projection, we omit the spin index of the electron wave function. The wave functions satisfy the one-dimensional Dirac equation,

$$\hat{h}\psi = \left(\sigma_3 \frac{v_F}{i} \frac{d}{dx} + \sigma_1 \Delta(x) \right) \psi(x) = \varepsilon \psi(x) , \quad (3)$$

where σ_1 and σ_3 the Pauli matrices. For the applicability of the continuum description of electrons, the random variations in the hopping amplitudes have to be relatively small.

This model was first introduced by Keldysh.¹⁰ It was also considered in the context of the thermodynamical properties of quasi-one-dimensional charge-transfer salts,¹³ and has been applied to study the effect of disorder on the Peierls transition temperature,^{14,15} as well as the effect of quantum lattice fluctuations on the optical spectrum of Peierls materials.^{16–18} Recently it was used to describe the phase diagram of disordered spin-Peierls systems.⁷

In the remainder of this section we discuss the dependence of the spectrum of the single-electron eigenstates on the disorder strength. By $\rho(\varepsilon)$ we denote the disorder averaged density of states per unit length:

$$\rho(\varepsilon) = \frac{1}{L} \langle \text{Tr} \left[\delta(\hat{h} - \varepsilon) \right] \rangle , \quad (4)$$

where L is the chain length. Due to the charge conjugation symmetry of the Dirac Hamiltonian, the density of states is a symmetric function of energy:

$$\rho(-\varepsilon) = \rho(\varepsilon) . \quad (5)$$

We also introduce $N(\varepsilon)$, equal to the average number of electronic states (per unit length) with energy between 0 and some $\varepsilon > 0$:

$$N(\varepsilon) = \int_0^\varepsilon d\varepsilon' \rho(\varepsilon') . \quad (6)$$

An analytical expression for $N(\varepsilon)$ was found by Ovchinnikov and Erikhman¹³ by means of the “phase formalism”,^{11,19}

$$N(\varepsilon) = \frac{2A}{(\pi v_F)^2} \frac{1}{(J_\nu^2(z) + N_\nu^2(z))} . \quad (7)$$

Here, $z = v_F \varepsilon / A$ and $\nu = v_F \Delta_0 / A$ are dimensionless variables, and $J_\nu(z)$ and $N_\nu(z)$ are, respectively, Bessel and Neumann functions.

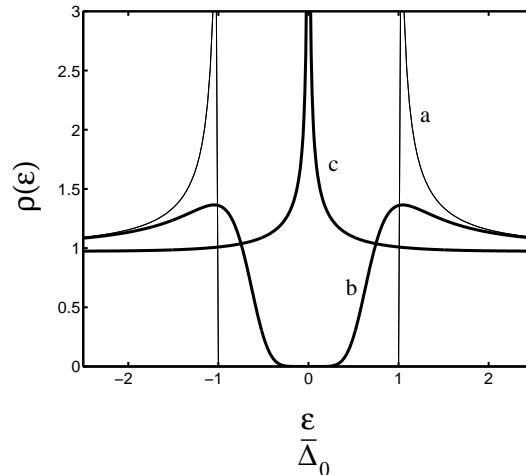


FIG. 1. Disorder-averaged density of states $\rho(\varepsilon)$ in the FGM for three values of the dimensionless disorder strength: $g = 0$, *i.e.*, no disorder (curve a), $g = 0.25$ (curve b), $g = 4$ (curve c). The free electron density of states was set to unity.

In Fig.1 we plot the average density of states $\rho(\varepsilon)$ for several values of the dimensionless disorder strength $g = 1/\nu = A/(v_F \Delta_0)$. In the absence of disorder ($\Delta(x) = \Delta_0$), the electron spectrum has a gap between the energies $\varepsilon = -\Delta_0$ and $\varepsilon = +\Delta_0$. Disorder gives rise to the appearance of electron states inside the gap. The energy dependence of the average density of states close to the Fermi energy ($|\varepsilon| \ll \Delta_0$) is given approximately by¹³

$$\rho(\varepsilon) = \frac{2}{v_F g \Gamma^2(\frac{1}{g})} \left(\frac{\varepsilon}{2g\Delta_0} \right)^{\frac{2}{g}-1} \quad (8)$$

(here and below we assume ε to be positive, which is sufficient in view of Eq.(5)). For $g < 2$ the density of states has a pseudogap (the Peierls gap filled with disorder-induced states). For $g > 2$ the pseudogap disappears and the density of states becomes divergent at $\varepsilon = 0$. This is a Dyson-type singularity,²⁰ which occurs in the band center for random Hamiltonians with charge conjugation symmetry.

In Ref. 5 we showed that the energy-dependence of the average density of states at small energy and weak disorder is mainly determined by the weight of the optimal disorder fluctuation $\bar{\eta}(x)$, which is defined as the most probable among the fluctuations that induce a state at given energy ε . The form of the optimal fluctuation is

$$\bar{\eta}(x) = -v_F K \left[\tanh \left(K(x - x_0 + \frac{R}{2}) \right) - \tanh \left(K(x - x_0 - \frac{R}{2}) \right) \right] , \quad (9)$$

where x_0 and R describe, respectively, the position and the spatial extent of the disorder fluctuation, and K is determined by

$$v_F K = \Delta_0 \tanh(KR) . \quad (10)$$

Thus, $\Delta(x) = \Delta_0 + \bar{\eta}(x)$, plotted in Fig. 2, has precisely the form of a soliton-antisoliton pair discussed in Refs. 21,22 in the context of polaron excitations in the conjugated polymer *trans*-polyacetylene. The

spectrum of electron states for this $\Delta(x)$ (also plotted in Fig. 2) consists of a valence band (with highest energy $-\Delta_0$), a conduction band (with lowest energy $+\Delta_0$), and two localized intragap states $\psi_{\pm}(x)$ with energies $\pm\varepsilon_0(R)$, where

$$\varepsilon_0(R) = \frac{\Delta_0}{\cosh(KR)} . \quad (11)$$

The soliton-antisoliton separation R is fixed by the condition $\varepsilon_0(R) = \varepsilon$. The two intragap states are the symmetric and antisymmetric superpositions of the midgap states localized near the soliton and antisoliton.¹² The energy splitting 2ε decreases exponentially with the soliton-antisoliton separation, so that for $\varepsilon \ll \Delta_0$,

$$R \approx \xi_0 \ln \frac{2\Delta_0}{\varepsilon} , \quad (12)$$

where $\xi_0 = v_F/\Delta_0$ is the correlation length.

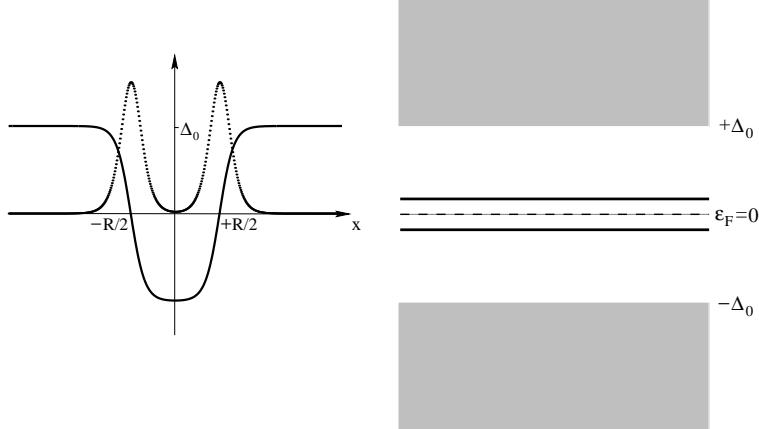


FIG. 2. The left part of the picture shows $\Delta(x) = \Delta_0 + \bar{\eta}(x)$ for the instanton disorder fluctuation (thick line) and the electron density $|\psi_+(x)|^2 = |\psi_-(x)|^2$ for the corresponding intragap states (dotted line); the right part of the picture shows the spectrum of electron states for the optimal disorder fluctuation.

For white-noise disorder with the correlator Eq.(2), the weight $p[\eta(x)]$ of the disorder configuration $\eta(x)$ is given by

$$p[\eta(x)] = \exp \left(-\frac{1}{2A} \int dx \eta^2(x) \right) . \quad (13)$$

Using Eq.(12) we find that the weight of the optimal configuration,

$$p[\bar{\eta}(x)] \propto \varepsilon^{\frac{2}{g}} , \quad (14)$$

gives, indeed, a good estimate for the shape of the density of states inside the pseudogap for $g \ll 1$ [cf. Eq.(8)].

We would like to conclude this section by noting that, while in the random potential problem the optimal fluctuation induces one state with large negative energy,¹⁻³ in the FGM the soliton-antisoliton fluctuation Eq.(9) induces two states with energies $\pm\varepsilon$. The small difference between the energies of the symmetric and antisymmetric states is potentially dangerous for the application of the optimal fluctuation method to the FGM. The problem arises in the calculation of the contribution of the disorder realizations close to the optimal fluctuation:

$$\eta(x) = \bar{\eta}(x) + \delta\eta(x) .$$

The perturbation $\delta\hat{h} = \sigma_1 \delta\eta(x)$ can, in principle, strongly mix the symmetric and antisymmetric intragap states, because of the small energy denominator 2ε appearing in the perturbation series. Such mixing would affect the value of the energy splitting between the two states. This problem arises because of

the charge conjugation symmetry of the Dirac Hamiltonian Eq.(3), which implies the symmetry of the spectrum of its eigenvalues around $\varepsilon = 0$. We address this question in Appendix A, where we show that, just because of the symmetry of the Hamiltonian Eq.(3), the mixing of the symmetric and antisymmetric states is small and thus, despite the small energy splitting, the optimal fluctuation method is applicable. The result of Appendix A also justifies our calculation of the optical absorption coefficient presented in Ref. 5.

III. FUNCTIONAL INTEGRATION

The weight of the optimal fluctuation, given by Eq.(14), is the main factor that describes the suppression of the density of states at small energy. To obtain a full expression for the density, however, one has to take into account the contribution of the disorder realizations close to the optimal configuration. In this section we perform this calculation using the correspondence between the averaging over disorder realizations $\eta(x)$ and the quantum-mechanical averaging over the ground state for a certain double-well potential. Then the main suppression factor Eq.(14), as well as the correction to it, can be easily found using well-known methods developed for the double-well problem.

A. The corresponding quantum-mechanical problem

The density of electron states averaged over the white-noise disorder can be written in the form of the functional integral:

$$\rho(\varepsilon) = \frac{1}{L} \int D\eta(x) \exp \left(-\frac{S}{A} \right) \text{Tr} \left[\delta(\hat{h} - \varepsilon) \right], \quad (15)$$

with

$$S = \frac{1}{2} \int_{-L/2}^{L/2} dx \eta^2(x), \quad (16)$$

and \hat{h} as defined in Eq.(3). The relation between the functional integral and a particular quantum mechanical problem will become apparent after we make a substitution of variables that allows us to express the disorder fluctuation $\eta(x)$ in terms of the eigenfunction $\psi(x)$ of Eq.(3) with energy ε . Due to time-reversal symmetry of the Dirac Hamiltonian its eigenfunctions $\psi(x)$ can be chosen to satisfy

$$\sigma_1 \psi(x) = \psi(x), \quad (17)$$

and, therefore, can be written in the form:

$$\psi = \begin{pmatrix} u \\ u^* \end{pmatrix}. \quad (18)$$

The two real variables w and ϕ introduced by

$$u = w (\cosh(\phi) + i \sinh(\phi)), \quad (19)$$

then satisfy,

$$-v_F \frac{d\phi}{dx} + \varepsilon \cosh(2\phi(x)) - \Delta_0 = \eta(x), \quad (20)$$

and

$$v_F \frac{d \ln w(x)}{dx} = -\varepsilon \sinh(2\phi(x)). \quad (21)$$

We now use Eq.(20) to express the disorder configuration $\eta(x)$ in terms of $\phi(x)$. Then S , defined by Eq.(16), can be written as

$$S[\phi(x)] = S_E[\phi(x)] + S_B , \quad (22)$$

where

$$S_E[\phi(x)] = \frac{1}{2} \int_{-L/2}^{L/2} dx \left(v_F^2 \left(\frac{d\phi}{dx} \right)^2 + (\Delta_0 - \varepsilon \cosh(2\phi))^2 \right) , \quad (23)$$

and

$$S_B = \frac{1}{2} v_F (2\Delta_0 \phi - \varepsilon \sinh(2\phi)) \Big|_{-L/2}^{+L/2} . \quad (24)$$

$S_E[\phi(x)]$ has the form of the Euclidean action of a particle with mass v_F^2 and coordinate ϕ moving in the imaginary time x in the inverted double-well potential,

$$U(\phi) = -\frac{\Delta_0^2}{2} \left(1 - \frac{\cosh(2\phi)}{\cosh(2\varphi)} \right)^2 , \quad (25)$$

plotted in Fig. 3. The angle φ in Eq.(25) is defined by

$$\cosh(2\varphi) = \frac{\Delta_0}{\varepsilon} . \quad (26)$$

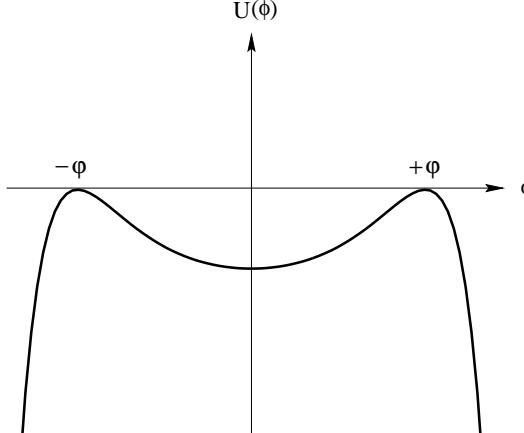


FIG. 3. The inverted double-well potential $U(\phi)$. The instanton trajectory starts at the left maximum $-\varphi$ and ends at the right maximum $+\varphi$.

Finally, in the functional integral Eq.(15), the disorder strength A plays the role of \hbar . Thus, we have identified the quantum double-well problem that corresponds to our disorder average. A similar correspondence exists also for the random potential problem.²³

B. The instanton solution

The instanton $\bar{\phi}(x)$ is the solution of the classical equation of motion in the inverted double-well potential with the boundary conditions

$$\bar{\phi}(\pm\infty) = \pm\varphi . \quad (27)$$

This corresponds to infinitely long motion from the left maximum to the right one. The energy on this classical trajectory,

$$E = \frac{v_F^2}{2} \left(\frac{d\bar{\phi}}{dx} \right)^2 - U(\bar{\phi}) , \quad (28)$$

equals zero, which gives,

$$v_F \frac{d\bar{\phi}}{dx} = \pm (\Delta_0 - \varepsilon \cosh(2\bar{\phi}(x))) . \quad (29)$$

As the solution with the minus sign corresponds to the trivial disorder configuration $\eta(x) = 0$ [cf. Eq.(20)], we choose the plus sign. Equation (29) is easily solved, yielding

$$e^{2\bar{\phi}(x)} = \frac{\cosh(K(x - x_0 + \frac{R}{2}))}{\cosh(K(x - x_0 - \frac{R}{2}))} , \quad (30)$$

where K and R are defined by

$$K = \frac{\Delta_0}{v_F} \tanh(2\varphi) , \quad (31)$$

and

$$KR = 2\varphi . \quad (32)$$

Using Eq.(20) we find that the instanton Eq.(30) is exactly the optimal disorder configuration given by Eq.(9) and that Eqs. (26), (31), and (32) defining the parameters of the instanton solution coincide with Eqs. (10) and (11). Finally, for the instanton trajectory, the value of S defined by Eq.(22) is:

$$\frac{S_0}{A} = \frac{S[\bar{\phi}(x)]}{A} = \frac{2}{g} (2\varphi - \tanh(2\varphi)) . \quad (33)$$

C. Boundary conditions

We note that the boundary conditions Eq.(27) for the instanton trajectory are not, in general, the boundary conditions that one usually imposes on the eigenfunction $\psi(x)$. In particular, φ defined by Eq.(26), depends on the energy ε , while, for instance, the boundary conditions for a finite Peierls chain with an even number of atoms in the continuum limit take the form²⁴

$$\frac{\text{Im}(u(\pm L/2))}{\text{Re}(u(\pm L/2))} = \pm 1 , \quad (34)$$

which is equivalent to

$$\phi_{R,L} = \phi|_{\pm L/2} = \pm\infty . \quad (35)$$

We discuss the instanton for these boundary conditions in Appendix B. It is clear, however, that in the limit $L \rightarrow \infty$ the density of states should not depend on the boundary conditions. Therefore, we choose here the ones that lead to the easiest calculation of the density of states, namely,

$$\phi_{R,L} = \bar{\phi}\left(\pm \frac{L}{2}\right) , \quad (36)$$

where $\bar{\phi}(x)$ is the instanton solution given by Eq.(30) with $x_0 = 0$. With the last condition $\bar{\phi}(x)$ is antisymmetric, so that

$$\phi_L = -\phi_R . \quad (37)$$

D. Regularization

In order to perform the functional integration in Eq.(15), we first have to regularize it. We do this by dividing the range of variation of x , $[-\frac{L}{2}, \frac{L}{2}]$, into N small intervals of size a , assuming the value of η to be constant inside each interval. Then,

$$\frac{1}{2A} \int_{-L/2}^{L/2} dx \eta^2(x) = \frac{a}{2A} \sum_{n=1}^N \eta_n^2 , \quad (38)$$

and the integration measure,

$$D\eta(x) = \prod_{n=1}^N \frac{d\eta_n}{\left[\frac{2\pi A}{a}\right]^{\frac{1}{2}}} , \quad (39)$$

is defined in such a way that the average of the unity operator is one.

In the regularized version of the substitution Eq.(20), the new variables ϕ_n ($n = 1, \dots, N$) are the values of ϕ on the right end of each interval and

$$\phi_0 = \phi_L , \quad (40)$$

is fixed by the boundary condition at the chain's left end. For the moment we treat Eq.(20) as a functional substitution and forget about the boundary condition at the right end. Up to second order in a , the regularized form of the substitution reads:

$$v_F \frac{(\phi_n - \phi_{n-1})}{a} = \frac{(\varepsilon \cosh(2\phi_{n-1}) - \Delta_0 - \eta_n)}{\left(1 - \frac{a\varepsilon}{v_F} \sinh(2\phi_{n-1})\right)} . \quad (41)$$

It is necessary to retain the higher order term in powers of a for the correct calculation of the Jacobian of the substitution. The integration measure can now be written as

$$D\eta(x) = \prod_{n=1}^N \frac{v_F d\phi_n}{[2\pi a A]^{\frac{1}{2}}} J , \quad (42)$$

with

$$J = \prod_{n=1}^N \left(1 - \frac{a\varepsilon}{v_F} \sinh(2\phi_{n-1})\right) \approx \exp\left(-\frac{\varepsilon}{v_F} \int_{-L/2}^{L/2} dx \sinh(2\phi(x))\right) . \quad (43)$$

It is important that Eq.(41) provides a one-to-one correspondence between the disorder configuration $\{\eta_n\}$ and the values of the solution of the differential equation (20) at the points $x = an$, $n = 1, \dots, N$. In other words, Eq.(41) relates the disorder configuration to the electron wave function in the presence of this disorder, which gives us a convenient representation for the trace of the delta-dunction in Eq.(15). The energy ε is the eigenvalue of the Hamiltonian \hat{h} if ϕ at the right end satisfies the boundary condition:

$$\phi_N = \phi_R . \quad (44)$$

Therefore, the average density of states Eq.(15) can be written in the form:

$$\rho(\varepsilon) = \frac{1}{L} \int D\eta(x) \exp\left(-\frac{S}{A}\right) \left(\frac{\partial \phi_N}{\partial \varepsilon}\right)_{\phi_0, \eta(x)} \delta(\phi_N - \phi_R) . \quad (45)$$

The delta-function removes the integration over ϕ_N and, using Eq.(20), one can easily calculate the derivative of ϕ_N with respect to ε , keeping both the disorder $\eta(x)$ and the value of ϕ at the left end of the chain fixed:

$$\left(\frac{\partial \phi_N}{\partial \varepsilon}\right)_{\phi_0, \eta(x)} = \frac{y(\frac{L}{2})}{v_F} \int_{-L/2}^{L/2} dx \frac{\cosh(2\phi(x))}{y(x)} . \quad (46)$$

Here, $y(x)$ is given by

$$y(x) = \exp\left(\frac{2\varepsilon}{v_F} \int_{-L/2}^x dx' \sinh(2\phi(x'))\right) , \quad (47)$$

so that J , defined by Eq.(43), can be written as

$$J = \frac{1}{\sqrt{y\left(\frac{L}{2}\right)}}. \quad (48)$$

We thus arrive at the following final form of the functional integral

$$\rho(\varepsilon) = \frac{1}{L} \int D'\phi(x) \exp\left(-\frac{S_E}{A}\right) F[\phi(x)], \quad (49)$$

where the integration measure is defined by

$$D'\phi(x) = \frac{v_F}{[2\pi aA]^{\frac{1}{2}}} \prod_{n=1}^{N-1} \frac{v_F d\phi_n}{[2\pi aA]^{\frac{1}{2}}}, \quad (50)$$

and

$$F[\phi(x)] = J \left(\frac{\partial \phi_N}{\partial \varepsilon} \right)_{\phi_0, \eta(x)} \exp\left(-\frac{S_B}{A}\right). \quad (51)$$

E. Saddle-point integration

In this section we perform the functional integration in Eq.(49) over configurations $\phi(x)$ in the vicinity of the saddle-point configuration $\phi_{\text{sp}}(x)$ defined as

$$\left. \frac{\delta S}{\delta \phi(x)} \right|_{\phi_{\text{sp}}(x)} = 0. \quad (52)$$

The boundary conditions Eq.(36) were chosen to ensure that $\phi_{\text{sp}}(x) = \bar{\phi}(x)$, where $\bar{\phi}(x)$ is given by Eq.(30) with $x_0 = 0$.

The result of the integration is:

$$\rho(\varepsilon) = \frac{JD}{L} \left(\frac{\partial \phi_N}{\partial \varepsilon} \right)_{\phi_0, \bar{\eta}(x)} \exp\left(-\frac{S_0}{A}\right), \quad (53)$$

where S_0 is given by Eq.(33) and D is the determinant of the operator

$$-\frac{v_F^2}{2} \frac{d^2}{dx^2} + 4\varepsilon (\varepsilon \cosh(4\phi(x)) - \Delta_0 \cosh(2\phi(x))), \quad (54)$$

obtained by the second variation of the Euclidean action Eq.(23). In Eq.(53) J , D , and $\partial \phi_N / \partial \varepsilon$ have to be calculated at $\phi(x) = \bar{\phi}(x)$.

Using Eq.(29) (with the plus sign) one easily finds that

$$\frac{2\varepsilon}{v_F} \sinh(2\bar{\phi}) = -\frac{d}{dx} \ln \left(\frac{d\bar{\phi}}{dx} \right), \quad (55)$$

so that Eq.(47) can be written in the form

$$y(x) = \frac{\frac{d\bar{\phi}}{dx} \left(-\frac{L}{2}\right)}{\frac{d\bar{\phi}}{dx}(x)}. \quad (56)$$

Since $\bar{\phi}(x)$ is antisymmetric, $y\left(\frac{L}{2}\right) = 1$, so that $J = 1$ and

$$\left(\frac{\partial \phi_N}{\partial \varepsilon} \right)_{\phi_0, \bar{\eta}(x)} = \frac{\sinh(2\bar{\phi}\left(\frac{L}{2}\right))}{v_F \frac{d\bar{\phi}}{dx}\left(\frac{L}{2}\right)}. \quad (57)$$

As for large L , $\sinh(2\bar{\phi}(\frac{L}{2}))$ can be replaced by $\sinh(2\varphi)$ and

$$\frac{d\bar{\phi}}{dx} \left(\frac{L}{2} \right) \approx 2K \sinh(2\varphi) e^{-KL}, \quad (58)$$

we obtain

$$\left(\frac{\partial \phi_N}{\partial \varepsilon} \right)_{\phi_0, \bar{\eta}(x)} = \frac{e^{KL}}{2v_F K}. \quad (59)$$

We calculate the determinant D using the standard method for calculation of determinants of Schrödinger operators in one dimension, which can be found in Ref. 9. The result is

$$D = L \frac{(2Kv_F)^2}{\pi A} \sinh(2\varphi) e^{-KL}. \quad (60)$$

The determinant is proportional to the chain size, because the soliton-antisoliton pair can appear at any place in the chain (formally the factor L comes from the integration over the zero mode⁹). Taking all factors together, we finally obtain for the averaged density of states

$$\rho(\varepsilon) = \frac{2Kv_F}{\pi A} \sinh(2\varphi) \exp\left(-\frac{S_0}{A}\right). \quad (61)$$

The resulting expression for the average density of electron states in the limit $\varepsilon \ll \Delta_0$ is

$$\rho(\varepsilon) = \frac{e}{\pi g v_F} \left(\frac{e\varepsilon}{2\Delta_0} \right)^{\frac{2}{g}-1}. \quad (62)$$

For $g \ll 1$, this agrees with Eq.(8), confirming the validity of the optimal fluctuation method at small energies and weak disorder.

IV. DISCUSSION

In this paper, we have used functional integration to establish a relation between the Fluctuating Gap Model, which describes one-dimensional electron motion in the presence of both a Peierls distortion and quenched disorder, and the quantum motion of a particle in a double-well potential. Averaging over disorder realizations in the model with quenched disorder corresponds to the sum over all paths in the quantum-mechanical problem. We have shown that the instanton trajectory describing the imaginary-time motion between the two wells corresponds to the optimal disorder fluctuation. The probability of this fluctuation determines the asymptotic behavior of the averaged electron density of states.

We showed that the most probable form of the wave function of the electron states lying deep within the pseudogap contains two peaks. The optimal disorder fluctuation that induces such a state, has the form of a soliton-antisoliton pair and the peaks of the wave function are localized near the two kinks of this fluctuation (see Fig. 2). As we demonstrated in this paper and in Ref. 5, the instanton approach allows for a relatively easy calculation of the density of states and absorption coefficient. Our result Eq.(62) is valid if the density of disorder-induced states is small, which is the case when $|\varepsilon| \ll \Delta_0$ and $g \ll 1$.

Above, we emphasized the strong relation between the calculation of the disorder average and the double-well problem. However, there is also a clear difference: In the double-well problem, an important role is played by multi-instanton configurations, in which instantons are followed by anti-instantons and *vice versa*.⁹ Although the action for the configuration containing n instantons and anti-instantons is n times the action of a single instanton S_{inst} , the multi-instanton contribution obtains a factor $T^n/n!$ from the sum over all possible instanton positions (T is the imaginary time corresponding to L). This statistical factor grows with T , while the suppression factor $\exp(-nS_{\text{inst}}/\hbar)$ does not decrease any further, making the multi-instanton configurations important at large enough T . We note that it is the sum over all possible numbers of instantons and anti-instantons that gives the energy splitting between the two lowest states in the double-well potential.⁹

By contrast, the asymptotic expression Eq.(62) for the density of states in the FGM is given by only one instanton, which means that the largest contribution to the averaged density of states comes from a single disorder fluctuation. The origin of the difference lies in the fact that, while in the quantum double-well problem the anti-instanton describes a real physical process (the tunneling between the wells in the direction opposite to the one described by the instanton), in the FGM it corresponds to zero disorder. To see this, we note that the instanton $\phi_a(x) = \bar{\phi}(-x)$, obtained from the instanton by “time-reversal”, $x \rightarrow -x$, is the solution of Eq.(29) with the minus sign. Comparing this equation with Eq.(20), we find that $\phi_a(x)$ corresponds to $\eta(x) = 0$. The Euclidean action S_E of the anti-instanton is exactly cancelled by the “boundary” term S_B [cf. Eq.(22)]. It is then clear, that anti-instantons (and, hence, the multi-instanton configurations) cannot play any role for the calculation of the density of states. Formally, this happens because for $\phi(x) = \phi_a(x)$ we have:

$$\left(\frac{\partial \phi_N}{\partial \varepsilon} \right)_{\phi_0, \bar{\eta}(x)} \approx \frac{\Delta_0}{v_F K \varepsilon} + \frac{2LK}{\varepsilon} e^{-KL} , \quad (63)$$

which tends to a constant value in the large L limit, while the corresponding expression for the instanton solution Eq.(59) diverges as $\exp(KL)$. Since the value of the determinant $D \propto L \exp(-KL)$ for the anti-instanton is the same as for the instanton, the anti-instanton contribution is proportional to $L \exp(-KL)$ and, therefore, vanishes in the $L \rightarrow \infty$ limit.

ACKNOWLEDGEMENTS

The authors are grateful to Dr. I. V. Kolokolov for useful discussions. This work is supported by the “Stichting Scheikundig Onderzoek in Nederland (SON)” and the “Stichting voor Fundamenteel Onderzoek der Materie (FOM)”.

APPENDIX A: THE ROLE OF SYMMETRIES OF THE FGM HAMILTONIAN

In this appendix we show that owing to the symmetry properties of the FGM Hamiltonian a small perturbation of the optimal fluctuation

$$\eta(x) = \bar{\eta}(x) + \delta\eta(x) , \quad (A1)$$

does not strongly mix the symmetric and antisymmetric states, despite the small energy splitting between them. As was explained in Sec. II such a mixing, if it would occur, would invalidate our optimal fluctuation calculation.

First, we obtain the effective Hamiltonian, acting on the subspace of the two intragap states, which includes the virtual excitations to all other electron states. To this end we write the single-electron Hamiltonian for the disorder realization $\eta(x)$, given by Eq.(A1), in the form:

$$\hat{h} = \hat{h}^{(0)} + \hat{h}^{(1)} , \quad (A2)$$

where

$$\hat{h}^{(0)} = \sigma_3 \frac{v_F}{i} \frac{d}{dx} + \sigma_1 (\Delta_0 + \bar{\eta}(x)) , \quad (A3)$$

and $\hat{h}^{(1)}$ is the perturbation:

$$\hat{h}^{(1)} = \sigma_1 \delta\eta(x) . \quad (A4)$$

We divide the Hilbert space of the Hamiltonian $\hat{h}^{(0)}$ into two subspaces: A and B. The subspace A consists of the symmetric and antisymmetric intragap states, which here are denoted as $|\pm\rangle$, while all the other states belong to the subspace B, so that

$$\hat{P}_A + \hat{P}_B = 1 , \quad (A5)$$

where $\hat{P}_{A,B}$ are the projection operators for the corresponding subspaces. The effective energy-dependent Hamiltonian, acting on the subspace A, has the form:

$$\hat{h}_A(\varepsilon) = \hat{h}_A^{(0)} + \hat{h}_A^{(1)} + \hat{h}_A^{(v)}(\varepsilon) \quad (\text{A6})$$

where the first term is the diagonal 2-by-2 matrix:

$$\hat{h}_A^{(0)} = \hat{P}_A \hat{h}^{(0)} \hat{P}_A = \begin{pmatrix} +\varepsilon_0(R) & 0 \\ 0 & -\varepsilon_0(R) \end{pmatrix}, \quad (\text{A7})$$

the second term is the first-order perturbation,

$$\hat{h}_A^{(1)} = \hat{P}_A \hat{h}^{(1)} \hat{P}_A, \quad (\text{A8})$$

and the last term,

$$\hat{h}_A^{(v)}(\varepsilon) = \hat{P}_A \hat{h}^{(1)} \frac{1}{\varepsilon - \hat{h}^{(0)} - \hat{P}_B \hat{h}^{(1)}} \hat{P}_B \hat{h}^{(1)} \hat{P}_A, \quad (\text{A9})$$

describes the higher-order processes involving virtual excitations to the subspace B.

We now want to show that the non-diagonal matrix elements of the effective Hamiltonian $\hat{h}_A(\varepsilon)$ are smaller than its diagonal matrix elements. First, we show that the first-order nondiagonal matrix elements equal 0: On the one hand, using the relation $\psi_{\pm}^*(x) = \sigma_1 \psi_{\pm}(x)$ [cf. Eq.(17)] we obtain that the first-order perturbation Hamiltonian is real and symmetric:

$$\langle + | \hat{h}^{(1)} | - \rangle = \langle + | \sigma_1 \hat{h}^{(1)} \sigma_1 | - \rangle = \langle + | \hat{h}^{(1)} | - \rangle^* = \langle - | \hat{h}^{(1)} | + \rangle. \quad (\text{A10})$$

On the other hand, we can use the relation between the positive-energy and negative-energy eigenstates of the Dirac Hamiltonian, $\psi_{\pm}(x) = -\sigma_2 \psi_{\mp}(x)$, to show that

$$\langle + | \hat{h}^{(1)} | - \rangle = -\langle + | \sigma_2 \hat{h}^{(1)} \sigma_2 | - \rangle = -\langle - | \hat{h}^{(1)} | + \rangle. \quad (\text{A11})$$

Comparing Eq.(A10) with Eq.(A11) we obtain:

$$\langle + | \hat{h}^{(1)} | - \rangle = \langle - | \hat{h}^{(1)} | + \rangle = 0. \quad (\text{A12})$$

Next we consider the non-diagonal matrix elements of $\hat{h}_A^{(v)}(\varepsilon)$. The perturbative expansion of $\hat{h}_A^{(v)}(\varepsilon)$ in powers of $\hat{h}^{(1)}$ describes virtual excitations into the subspace B, so that all intermediate states in this expansion are separated from the intragap states by a large energy ($\gg \varepsilon_0(R)$). Since $|\varepsilon| \sim \varepsilon_0(R)$, the expansion terms involved do not contain small energy denominators. Moreover, the non-diagonal matrix elements of the operator (A9) equal 0 at $\varepsilon = 0$. The proof of this statement is analogous to the proof of Eq.(A12) and we shall not repeat it here.¹ Hence, the non-diagonal matrix elements of the operator $\hat{h}_A^{(v)}(\varepsilon)$ are $O(\varepsilon)$. Moreover, they contain an additional small factor $\delta\eta(x)/\Delta_0$. Therefore, the small disorder perturbation $\delta\eta(x)$ cannot result in a strong mixing of the two intragap states.

Next we show that the corrections to the energies of these two states due to the diagonal matrix elements of the effective Hamiltonian are also small, which will justify the validity of our calculation of the optical absorption coefficient.⁵ Using the expressions for the wave functions of the symmetric and antisymmetric states,⁵ the straightforward calculation of the first-order terms gives

$$\langle + | \hat{h}^{(1)} | + \rangle = -\langle - | \hat{h}^{(1)} | - \rangle = \int dx \delta\eta(x) \phi(x - \frac{R}{2}) \phi(x + \frac{R}{2}), \quad (\text{A13})$$

where

¹The important point is that in the basis of the eigenstates of $\hat{h}^{(0)}$, satisfying Eq.(17), $\hat{h}^{(0)}$ and $\hat{h}^{(1)}$ are real symmetric matrices and that they both anticommute with σ_2 .

$$\phi(x) = \sqrt{\frac{K}{2}} \frac{1}{\cosh(Kx)}. \quad (\text{A14})$$

Since the condition $\varepsilon_0(R) \ll \Delta_0$ implies $R \gg \xi_0$ [see Eq.(12)], the last equation can be written in the form:

$$\langle +|\hat{h}^{(1)}|+\rangle \approx \frac{2}{\xi_0} e^{-\frac{R}{\xi_0}} \int_{-R/2}^{R/2} dx \delta\eta(x) \approx \varepsilon_0(R) \int_{-R/2}^{R/2} \frac{dx}{\xi_0} \frac{\delta\eta(x)}{\Delta_0}, \quad (\text{A15})$$

i.e., the first-order correction to the energy of the intragap state with the energy $\pm\varepsilon_0(R)$ is proportional to this small energy times a factor $O\left(\frac{\delta\eta(x)}{\Delta_0}\right)$. This result can be easily traced back to the fact that the energy of the midgap state of a single kink cannot be changed by a small perturbation of $\Delta(x)$ (see, e.g., Ref. 25) and, therefore, it holds in all orders of the expansion of the effective Hamiltonian in powers of $\delta\eta(x)$.

Thus, we found that, despite the small energy splitting between the symmetric and antisymmetric intragap states, a small variation of the disorder fluctuation does not strongly affect either the wave functions, or the energies of these two states. This result is a direct consequence of symmetries of the Hamiltonian Eq.(3).

APPENDIX B: DIFFERENT BOUNDARY CONDITIONS

In this appendix we discuss the instanton trajectory for the boundary conditions Eq.(35), which one obtains in the continuum limit for an open chain with an even number of atoms. To avoid spurious divergences related to an infinite value of ϕ at the boundaries, we will use the following procedure. First, we impose, instead of Eq.(35), the boundary conditions,

$$\phi_{R,L} = \phi|_{\pm L/2} = \pm\Phi, \quad (\text{B1})$$

where $\Phi \gg \varphi$ is large but finite. Next we take the limit $L \rightarrow \infty$ and only then Φ is tended to infinity.

Since for $|\Phi| > \phi$ part of the instanton trajectory $\bar{\phi}(x)$ lies outside the well of the potential Eq.(25) located between $-\varphi$ and φ , the energy E defined by Eq.(28) is positive. For $E > 0$ the equation for the instanton trajectory is,

$$v_F \frac{d\bar{\phi}}{dx} = \sqrt{(\Delta_0 - \varepsilon \cosh(2\bar{\phi}(x)))^2 + 2E}. \quad (\text{B2})$$

Now, the particle's velocity becomes very large as soon as it leaves the well. The large Euclidean action Eq.(23) associated with this region is, however, completely compensated by the surface term Eq.(24) in the infinite L limit. To see this, one notes that even for infinite Φ the time of motion L along the instanton trajectory is finite, as the velocity grows very fast outside the well. We are, however, interested in long time (large L) trajectories. The only way to make L large is to tend the positive energy E to zero, in which case the particle would spend most of the time near the maxima $-\varphi$ and φ of the potential $U(\phi)$, where it has a small velocity. The relation between the energy and the time of motion for large L is,

$$E \approx 8 \frac{(Kv_F)^4}{\varepsilon^2} e^{-2\varphi} e^{-KL}. \quad (\text{B3})$$

For $\Phi \gg \varphi$ the dependence of the energy on Φ can be neglected.

When the energy E tends to zero, the trajectory given by Eq.(B2) inside the well, i.e., for $|\phi| < \varphi$, tends to the solution of Eq.(29) with the plus sign. In other words, in the limit $L \rightarrow \infty$, this part of the trajectory becomes the instanton solution Eq.(30) that we considered above. On the other hand, outside the well ($|\phi| > \varphi$) the solution of Eq.(B2) tends to the solution of Eq.(29) with the minus sign. The latter corresponds to zero disorder, $\eta(x) = 0$, which explains the cancellation between the Euclidean action coming from outside the well and the surface term. We proved, therefore, that in the limit $L \rightarrow \infty$ the suppression factor S for the instanton with boundary conditions Eq.(B1) is identical to Eq.(33).

The boundary conditions Eq.(B1) imply that the solution $\bar{\phi}(x)$ is antisymmetric. Therefore, the Jacobian J given by Eq.(48) equals unity, as before. At the same time, however, the values of the partial

derivative $\left(\frac{\partial\phi_N}{\partial\varepsilon}\right)_{\phi_0,\bar{\eta}(x)}$ and the determinant D differ considerably from Eqs. (59) and (60), respectively. For instance,

$$\left(\frac{\partial\phi_N}{\partial\varepsilon}\right)_{\phi_0,\bar{\eta}(x)} = \frac{e^{2\varphi} e^{4\Phi} e^{KL}}{16 \sinh^4(2\varphi)} . \quad (\text{B4})$$

Nevertheless, the product of the determinant and the partial derivative remains unchanged up to small corrections that vanish for $L \rightarrow \infty$. Therefore, despite the fact that the instanton trajectories for the boundary conditions Eq.(35) and Eq.(36) are rather different, the average density of states obtained by the saddle-point integration near these trajectories is the same for sufficiently long chains, as, of course, should be the case.

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